IN THE CLAIMS

1. (Currently amended) A method for the accurate determination of van der Waals parameters for high-precision determination of crystal structures and/or energies, comprising the steps of:

[[-]]numerically simulating at least one crystal structure based on density functional theory (DFT) calculations combined with a potential energy term representing Van der Waals interactions;

[[-]]providing reference data containing accurate information about said at least one crystal structure;

[[-]]defining a deviation function (F) quantifying a deviation between said reference data and said at least one simulated crystal structure;

[[-]]fitting at least one parameter of said van der Waals potential term in such a way as to minimize said deviation function (F); and

[[-]]obtaining the accurate van der Waals parameters from the best fit.

2. (Original) A method according to claim 1, characterized in that said van der Waals potential term is defined as:

$$E_{disp} = \sum_{A,B} - f_{A,B}(r_{A,B}) \frac{C_{6,A,B}}{R^{6}_{A,B}}$$

wherein $f_{A,B}$ $(r_{A,B})$ is a damping function and the sum runs over all pairs of interacting atoms, and that said fitting step comprises fitting said damping function.

3. (Original) A method according to claim 2, characterized in that said damping function is defined as

$$f_{A,B}(r) = \left(1 - \exp\left[-c\left(\frac{r}{r_{A,B}}\right)^{\frac{3}{n}}\right]\right)^{2n}$$

and that said fitting step comprises fitting the parameter $r_{A,B}$, and/or the parameter n and/or the parameter c.

4. (Currently amended) A method according to claim 2~~-or 3~~, characterized in that said fitting step furthermore comprises fitting said coefficient $C_{6,A,B}$.

5. (Currently amended) A method according to ~~any of the preceding claims~~claim 1, characterized in that said reference data are theoretical data obtained by Hartree-Fock calculations or Quantum Monte Carlo simulations.

6. (Currently amended) A method according to ~~any of the preceding claims~~claim 1, characterized in that said reference data are experimental low-temperature crystal structure data.

7. (Original) A method according to claim 6, characterized in that said crystal structure data are obtained by X-Ray or neutron scattering.

8. (Currently amended) A method according to claim 1 for the accurate determination of crystal structures and/or energies, comprising the steps of:

[[-]]providing a rough estimate model of at least one crystal structure;

[[-]]numerically simulating said at least one crystal structure based on density functional theory (DFT) calculations combined with a potential energy term representing Van der Waals interactions; and

[[-]]obtaining said at least one crystal structure and/or its energy as a result of said numerical simulation.[[,]]

~~characterized in that said van der Waals potential term is obtained by the method according to any of claims 1 to 7~~.

9. (Original) A method according to claim 8, characterized in that a plurality of polymorphic crystal structures are determined and ranked according to their respective energies.

10. (Original) A method for the efficient numerical optimization of a molecular crystal structure using an advantageous crystal coordinate system, comprising the steps of:

[[-]]providing a starting crystal lattice described by an initial coordinate system comprising lattice parameters and atomic positions in said crystal;

[[-]]defining a so-called natural coordinate system and representing said starting crystal lattice in said natural coordinate system, said natural coordinate system comprising:

- [[•]]first coordinates describing symmetry-allowed lattice changes and defined in such a way that changes of said first coordinates do not cause changes of the molecular geometry or a rotation of molecules with respect to each other and leave fractional coordinates of molecular centres constant;
- [[•]]second coordinates describing symmetry-allowed translations of said molecules in said crystal;
- [[•]]third coordinates describing symmetry-allowed rotations of said molecules in said crystal;
- [[•]]fourth coordinates describing symmetry-allowed changes of the molecular geometry;

[[-]]transforming coordinates from said natural coordinate system to said initial coordinate system;

[[-]]calculating the lattice energy and energy derivatives with respect to said initial coordinate system; and

[[-]]transforming said energy derivatives from said initial coordinate system to said natural coordinate system,

wherein a minimization algorithm is used for minimizing said lattice energy with respect to said natural coordinate system.

11. (Original) A method for the energy ranking of polymorphic crystal structures, comprising the steps of:

[[-]]providing rough estimate models of each of said crystal structures;

[[-]]numerically simulating each of said crystal structures based on density functional theory (DFT) calculations combined with a potential energy term representing Van der Waals interactions

[[-]]obtaining accurate crystal structures and energies as a result of said numerical simulation; and

[[-]]ranking said accurate crystal structures according to their respective accurate energies.

12. (Original) The method according to claim 11, characterized in that the crystals are crystals of pharmaceutical compounds.

13. (Original) The method according to claim 12, characterized in that it is applied to identify the most stable polymorphic form of a pharmaceutical compound.

14. (Currently amended) The method according to ~~any of claims 11 to 13~~ ~~, characterized in that it uses a method for the efficient optimization of the molecular crystal structure according to claim 10~~.

claim 11 including:

providing a starting crystal lattice described by an initial coordinate system comprising lattice parameters and atomic positions in said crystal;

defining a so-called natural coordinate system and representing said starting crystal lattice in said natural coordinate system, said natural coordinate system comprising:

first coordinates describing symmetry-allowed lattice changes and defined in such a way that changes of said first coordinates do not cause changes of the molecular geometry or a rotation of molecules with respect to each other and leave fractional coordinates of molecular centres constant;

second coordinates describing symmetry-allowed translations of said molecules in said crystal;

third coordinates describing symmetry-allowed rotations of said molecules in said crystal;

fourth coordinates describing symmetry-allowed changes of the molecular geometry;

transforming coordinates from said natural coordinate system to said initial coordinate system;

calculating the lattice energy and energy derivatives with respect to said initial coordinate system; and

transforming said energy derivatives from said initial coordinate system to said natural coordinate system,

wherein a minimization algorithm is used for minimizing said lattice energy with respect to said natural coordinate system.

15. (Currently Amended) ~~A computer program product comprising computer readable code for enabling a computer to perform a method according to any of the preceding claims when said code is executed.~~ The method according to claim 1 wherein the steps for determining the van der Waals parameters are performed by a computer program comprising computer readable code executable by a computer.

16. (New) The method according to claim 8 including providing a computer program comprising computer readable code executable by a computer that determines the crystal structures and/or energies.

17. (New) The method according to claim 10 including providing a computer program comprising computer readable code executable by a computer that numerically optimizes the molecular crystal structure.

18. (New) The method according to claim 11 including providing a computer program comprising computer readable code executable by a computer that energy ranks the polymorphic crystal structures.